dbLabCal V3

Administration

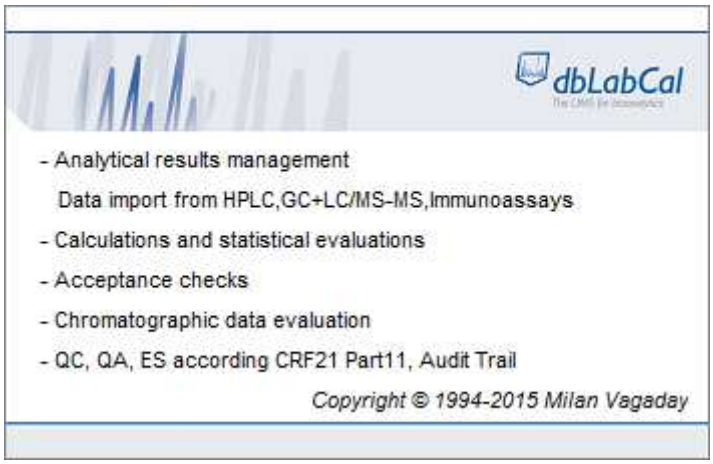


Table of Contents

1 Hardware and Software Requirements

dbLabCal V3 works with all current Oracle database versions. Recommended DBMS is Oracle12cR1, Oracle11gR2 or OracleXE (11g) and an Oracle11 client. The Oracle database may run on any server type (Windows, Unix, Linux etc.). Oracle database versions from 8.1.7 up to Oracle 12c were tested.

Hardware requirements for the database server:

	Minimum	Recommended
Processor	Intel (x86)	N/A
Memory	2 GB	4 GB or more
OS	W7 Pro or higher, 64bit or Windows Server 2008 R2	Windows Server 2008 R2 or Windows Server 2012 R2
Disk space	1.5 GB minimum	10 GB for Oracle and Data
Windows Installer	MSI version 2.0 minimum	N/A
Network	TCP/IP	N/A
Resolution	1024x768	N/A

For details see also:

Oracle 12c Release 1:
http://docs.oracle.com/database/121/index.htm

Oracle 11g Release 2 (11.2):
http://docs.oracle.com/cd/E11882_01/server.112/e10897/install.htm#ADMQS002

Oracle Database Express Edition 11g Release 2 (XE 11.2):
http://docs.oracle.com/cd/E17781_01/index.htm

dbLabCal V3 client runs on any computer which is suitable for Windows operating system. All current Windows versions up to Windows 8.1 were tested.
In addition, Oracle client software which is compatible with the used Oracle database (DBMS) version must be installed on each client PC. Recommended version is client version Oracle11g, the 32-bit version is mandatory.

Hardware requirements for the dbLabCal client:

	Minimum	Recommended
Processor	Intel (x86)	N/A
Memory	2 GB	4 GB
OS	Any Windows 7	W7 Pro or W8.1 Pro or higher, 64bit
Disk space	1.5 GB minimum	1.5 GB minimum
Resolution	1024x768	1980x1200

2 Installation

Full dbLabCal installation consists of following steps:

2.1. Oracle database installation on the database server
2.2. Oracle database configuration for dbLabCal (instance and/or schema creation)
2.3. dbLabCal schema configuration
2.4. copy dblabcal.exe plus config and license files into a shared folder
2.5. Oracle client (including OO4O) installation on each dbLabCal client PC
2.6. dbLabCal client package installation on each dbLabCal client PC
2.7. License file configuration
2.8. Initial configuration of dbLabCal database
(definition of departments, chromatographic systems and user in the database)

Perform steps 2.1-2.7 as administrator, step 2.8 as dbLabCal administrator

2.1 Oracle Database installation on the database server

Install Oracle DBMS version on the database server according Oracle's instructions.
No special requirements for dbLabCal exist.

Download links for Oracle Database 12c Release 1, Oracle Database 11g Release 2 or Oracle Database 11g Express Edition:
http://www.oracle.com/technetwork/database/enterprise-edition/downloads/index.html

2.2 Oracle Database configuration for dbLabCal (instance and/or schema creation)

2.2.1 Instance

Create new instance for dbLabCal with Oracle's Database Configuration Assistant (DCA). It is also possible to use any already existing instance. You may also create tablespaces for dbLabCal data or just use Oracle's defaults. The only requirement of dbLabCal is to having an own schema.
Check in DCA that following options are ON for the instance to be used by dbLabCal:

- Configure DB with EM
- Enable Daily Backup
- Flash Recovery Area
- Archiving
- EM Repository
- Character set is UTF8

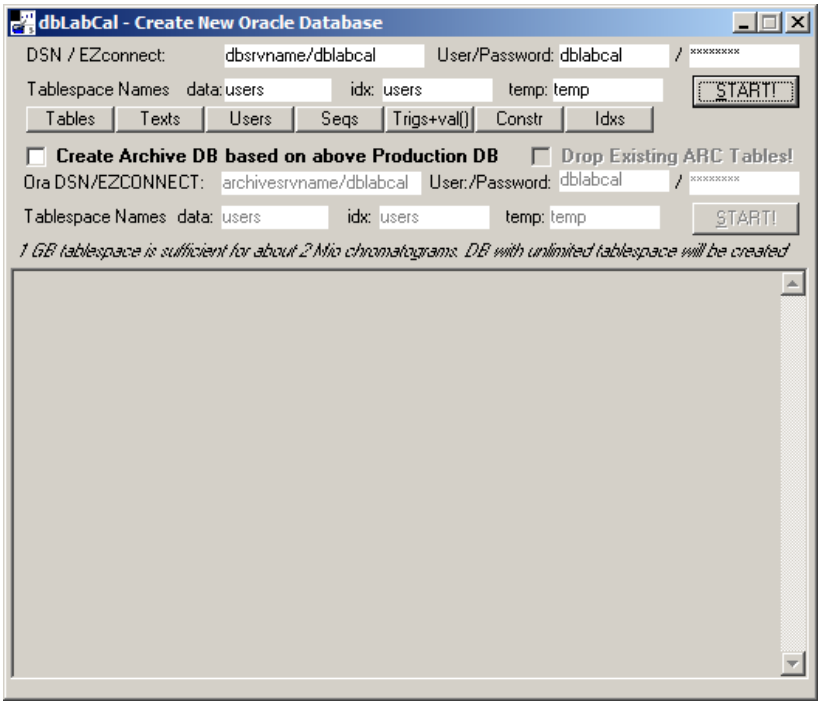
2.2.2 Schema (DBA user `dblabcal`)

Create the DBA user `dblabcal` e.g. by executing following 3 sql statements in sqlplus or sqldeveloper:

```
create user dblabcal identified by DBLABCAL;
grant DBA to dblabcal;
alter profile DEFAULT limit PASSWORD_LIFE_TIME UNLIMITED;
```

2.3 DBLABCAL Schema Configuration

All database objects required for dbLabCal are created with the tool `dbcreora.exe`. `dbcreora.exe` may be also helpful to re-create potentially corrupted objects like sequences, triggers, constraints or indexes.
Start dbcreora.exe from ...\dblabcal.v3\setup\create_dblabcal_schema\ folder and login as the DBA user `DBLABCAL` created in section 2.2.2. All required objects are created after click on the START! button.



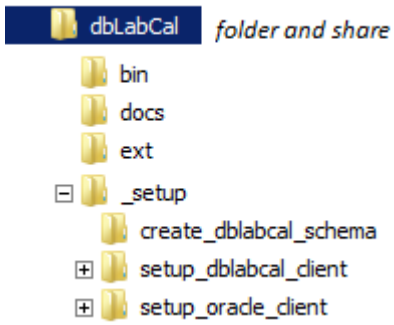
dbcreora.exe creates also another one DBA user (with USERID of the current Windows user) and grants dbLabCal administrator permissions to this user.

Check also the output in dbcreora.exe (dbcreora.log file) for details!

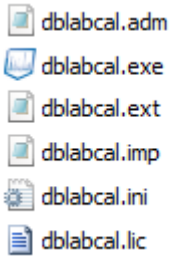
2.4 Copy dblabcal.exe into server share

Copy the content of the dbLabCal installation media into a share `dblabcal` created on the database server.

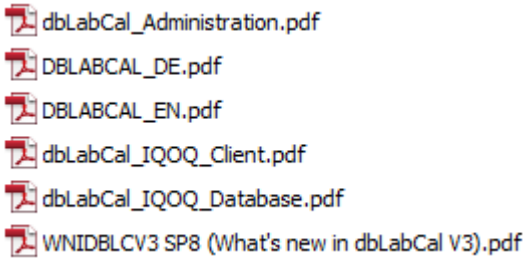
database server



bin folder



docs folder



2.5 Oracle Client installation (each client PC)

Start setup.exe (on each client PC) from ...\dblabcal_setup\setup_oracle_client\ to install the **32-bit** Oracle client.

Only the Oracle11g 32-bit client has Oracle Object for OLE (OO4O) required by the dbLabCal!

Select the `Administrator` option for the Oracle client installation.
Following item must be selected if for some reason `User defined` installation option is required:

- Oracle Object for OLE
- Oracle database utilities

2.6 dbLabCal Client installation (each client PC)

Start setup.exe (on each client PC) from ...\dblabcal_setup\setup_dblabcal_client\ and create shortcut to ...\dblabcal\bin\dblabcal.exe on the desktop

2.7 LIC File

Copy dbLabCal's license file `dblabcal.lic` together with the `dblabcal.ini` file ***)** into a shared folder on a server.

Oracle client (32-bit Oracle client!) must be installed on the database server in addition to the database components.

The path to the share of dblabcal.lic file is set in the dblabcal.adm (administration) file:

```
[Database]
…
lic=\\dbservername\dblabcal\   *)
…
```

Corresponding ini file has entries directing back to dblabcal.exe path and to the database instance:

```
[dblabcal]
path=\\appservername\exefoldername\dbLabCal\
db=dbservername/dblabcal
```

***)**
dblabcal.ini file is not required if dblabcal.exe, dblabcal.adm and dblabcal.lic are in same folder

2.8 Initial Configuration of dbLabCal database

- Login as administrator or an user with write permissions to ...\dblabcal.v3\bin\ folder
- Edit dblabcal.adm file in ...\dblabcal.v3\bin\ folder:
  Use easy connect naming `DBSERVERNAME/INSTANCENAME` to connect to the database or edit tnsnames.ora. tnsnames.ora is either local or on shared location (set global environment variable TNS_ADMIN to shared path).
  Example tnsnames.ora:

```
dblabcal =
  (DESCRIPTION =
    (ADDRESS_LIST =
      (ADDRESS = (PROTOCOL = TCP)(HOST = dbservername)(PORT = 1521))
    )
    (CONNECT_DATA =
      (SERVICE_NAME = DBLABCAL)
    )
  )
```

- Start dbLabCal V3
  Enter ORACLE ADMIN PASSWORD (password of the user DBA dblabcal)
- Enter ORACLE USER PASSWORD
  (Password of the user who has created dblabcal schema with dbcreora.exe. Password is by default dblabcal. Check also the dbcreora.log file)
- Edit Departments
- Edit Users

3 Maintenance

Only standard Oracle database maintenance procedures are required. Also, there is no need to work in Oracle database directly after database was once created and the database backup was established and checked.

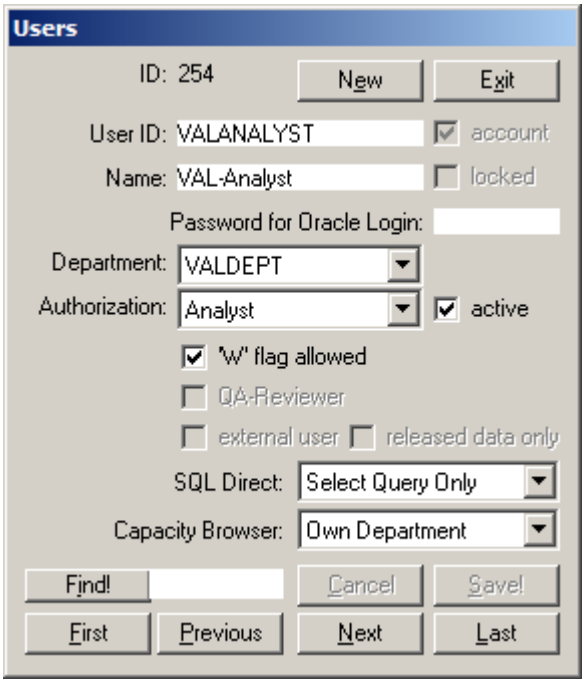
4 Administration

For additional information, see also the db menu chapter in dbLabCal User Manual.

4.1 User Account Administration

New Account

DB menu -> USERS... , NEW, edit user, finish with click on button SAVE...

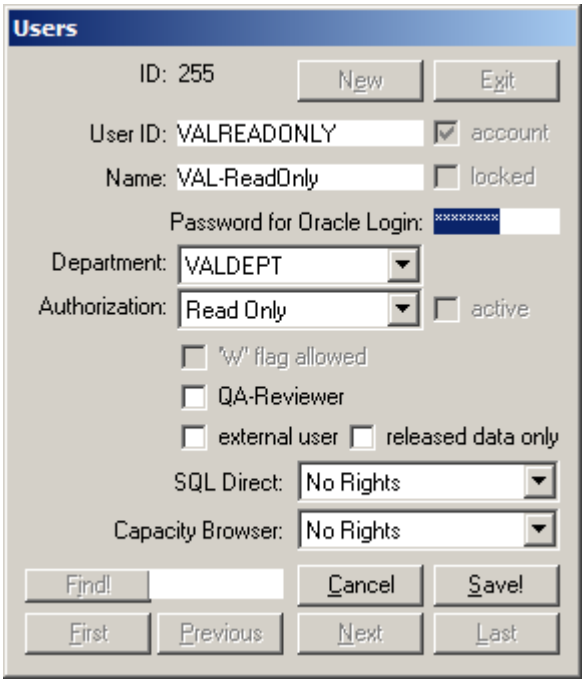


If the new user is not „ReadOnly“ user (means the user is involved in measurements) click the check box 

.

Change Account, Reset Password

DB menu -> USERS... , make changes in dialog, finish with click on button SAVE...



Lock / Unlock Account

User is locked by Oracle automatically after specific period of inactivity (locked timeout)
To unlock a user, proceed as described in Change Account (e.g. change password).
The account will be automatically unlocked when changing the users password.

4.2 User Groups Administration

dbLabCal users can be grouped in departments (groups).

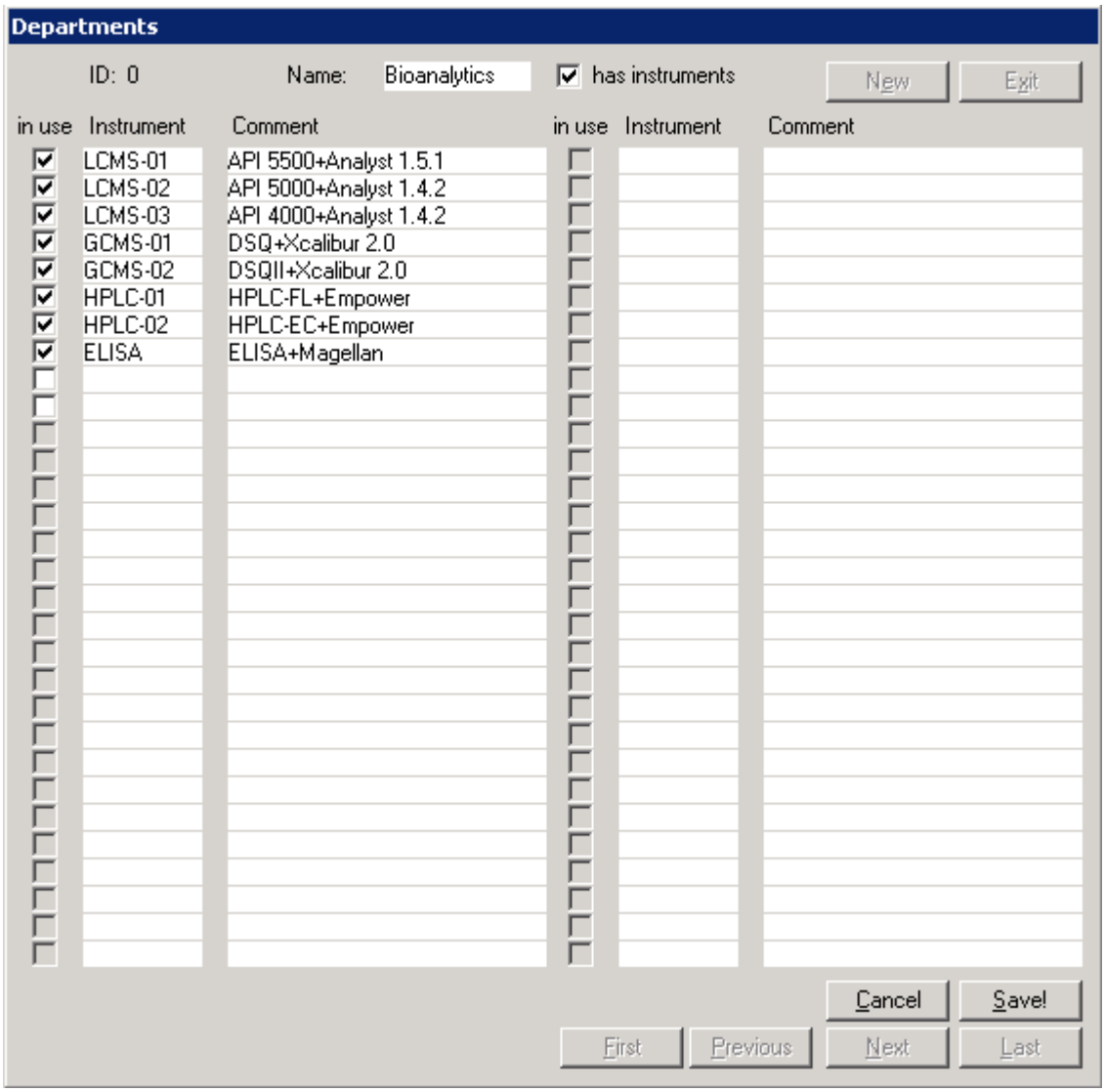
There are 6 fixed user types:

- ReadOnly
- Analyst
- Study Director/BPI
- Department Manager
- QA
- Administrator

Permissions for each User types cannot be further edited. For additional information, see User Authorization chapter in dbLabCal User Manual.

4.3 Department Administration

db menu -> Departments... , make changes in dialog, finish with click on button Save...
Check box ☑ has instruments means the department and the (selected) instruments will be showed-up in various dialogs for selection when editing projects in dbLabCal.
Furthermore, all users of the department can be set to not „active“ by deselecting the check box „has instruments“.



5 Appendix

5.1 SQD File Structure (for data import)

Line		Type		Content	*Comment*
1		text	*	**DBLABCAL SQD ASCII FILE**	*File Header (first line is fixed text to identify the file as dblabcals file)*
2		numeric	*	sequence (run) number	*Header Start*
3		text		Comment	
4		numeric	*	unit number	
5		text		analyst name	
6		text		sample preparation date	
7		text		sequence (run) start date	
8		text		sequence (run) end date	
9		text	*	study code	
10		text	*	Matrix	
11		numeric	*	peak count	
	*for **P**=1 to peak count*				
12		text	*	name of peak **P**	
	....	numeric		ID of peak **P**	
	next **P**				
#		numeric	*	Chromatogram count	*File Header End*
	*for **C**=1 to chromatogram count*				
#		text	*	Chromatogram file name	
#		text	*	sample type (TXTSYSIN, IDs 1-7)	*(CAL, QCS, SUB, VAL, DIV, EQC)*
#		text	+	subject number or subject name or sample name for DIV	*(SUB, DIV)*
#		numeric	+	period number	
#		text	+	Time expressed as: -number (e.g. 14=14 hours) or -dhm-Text (e.g. 3d2h30m=3 days, 2 hours, 30 minutes) or -hhh:mm-Text (e.g. 018:30=18 hours, 30 minutes)	*(SUB and/or VAL)*
#		text	+	Temperature (TXTSYSIN, IDs 11-15,)	*(VAL)*
#		Text	+	Matrix (TXTSYSIN, IDs 21-24)	*(VAL)*
#		numeric	*	Dilution factor	
#		Text		Remark to chromatogram	
#		numeric		Flag if chromatogram to be imported into database	
	*for **P**=1 to peak count*				
#		text	*	Chromatogram flag for peak **P** in chromatogram **C** (TXTSYSIN, IDs 31-39)	*(J/Y, N, S, V, A/E, X)*
#		numeric	+	Nominal conc. for peak **P** in chromatogram **C**	*(CAL, QCS, VAL)*
#		numeric	*	Retention time for peak **P** in chromatogram **C**	*if no peak; = 0*
#		numeric	*	area for peak **P** in chromatogram **C**	*if no peak; = 0*
#		numeric	*	Height for peak **P** in chromatogram **C**	*if no peak; = 0*
#		numeric	*	Retention time for IS for peak **P** in chromatogram **C**	*if no peak or IS not used; = 0*
#		numeric	*	area for IS for peak **P** in chromatogram **C**	*if no peak or IS not used; = 0*
#		numeric	*	Height for IS for peak **P** in chromatogram **C**	*if no peak or IS not used; = 0*
	next **P**				
	next **C**				

* *a value **must** be in this line*

\+ *may be left as blank line (if required, the data may be edited later in the database)*

5.2 ASCII File Structure (for data export)

This is the format of the plain ASCII file which contains the results of the subject samples. This ASCII file may be used to import the results into another applications, e.g. for biometrical calculations (SAS).

	Column 0 1 1234567890	2 1234567890	3 1234567890	4 1234567890	5 1234567890	6 1234567890
line						
1	**PROJECT...**	*XXXXXXXXXX*	*XXXXXXXXX.*	.....	.....	.....
2	**SPONSOR...**	*YYYYYYYYYY*	.....	.....	.....	.....
3	**GLPCODE...**	*ZZZZZZZZZZ*	.....	.....	.....	.....
4	**ANALYTE...**	*Analyte...*	*Name.....*	.....	.....	.....
5	**MATRIX....**	*Matrix....*	*Name.....*	.....	.....	.....
6	**COMMENT...**	*Comment.to*	*Project...*	.....	.....	.....
7	.....	*(blankline*)	.....	.....	.....	.....
8	.....	.....	**...SUBJECT**	**....PERIOD**	**...TIME[h]**	*.....ng/ml*
9	.....	.....	.....*1*	.....*1*	*.....0.000*	*.....<2.50*
10	.....	.....	.....*1*	.....*1*	*.....0.033*	*......19.2*
11	.....	.....	.....*1*	.....*1*	*.....0.083*	*......20.0*
12	.....	.....	.....*1*	.....*1*	*.....0.167*	*......20.7*
13	.....	.....	.....*1*	.....*1*	*.....0.250*	*......24.0*
14	.....	.....	.....*1*	.....*1*	*.....0.500*	*......48.6*
15	.....	.....	.....*1*	.....*1*	*.....0.750*	*......51.6*
16	.....	.....	.....*1*	.....*1*	*.....1.000*	*......NOS*
17	.....	.....	.....*1*	.....*1*	*.....2.000*	*......54.0*
18	.....	.....	.....*1*	.....*1*	*.....6.000*	*......55.9*
19	.....	.....	.....*1*	.....*1*	*...120.000*	*......56.7*
etc.						

NOS: no sample
NOA: sample not analyzed (received sample was not needed to be analyzed according to protocol, chromatogram flag was set to I)
NOR: result not reported (sample available and analyzed but no valid conc. result obtained)

5.3 dblabcal.adm File

dblabcal.adm is a control file for dblabcal.exe. It is used by dbLabCal V3 to login into the database and must be in the same folder as dblabcal.exe

The section entries are:

```
[Database]
oradsn= database connection (either tnsnames.ora or easyconnect)

[Admin]
name= Oracle schema(=Oracle user) used to store the data (default=DBLABCAL)
PWD= password for the Oracle schema(=Oracle user)

[Mill]
loginproject= name of valid/existing Empower project to login (to check users
Millennium password)
```

Examples....

```
[Database]
;Production (example easy connect)
oradsn=svrname/dblabcal
;DEV (example tnsnames.ora)
;oradsn=dblabcalDEV

[Admin]
name=DBLABCAL
PWD=8D0683C06C6A06……

[Mill]
loginproject=TEST
;loginproject must be a valid Empower project
;otherwise login errors in Import dialog
```

5.4 dblabcal.ini File

dblabcal.ini is a control file for dblabcal.lic. It is used to set dblabcal.exe location and the database connection. It is required for the license file.

The section entries are:

```
[dblabcal]
path=\\FILESERVERNAME\path_to_dblabcalexe\
db=DBSERVERNAME/INSTANCENAME
```

Examples....

```
[dblabcal]
path=\\FILESERVERNAME\dblabcal\bin\
db=DBSERVERNAME/XE
```

5.5 dblabcal.ext File

dblabcal.ext is a control file for dblabcal.exe.
dblabcal.ext is used by dbLabCal V3 to fill its Extra menu. Extra menu allows the user to start any application / document from dbLabCal directly. It saves few clicks
It can be missing, but if used, it must be in the same folder as dblabcal.exe

It has one fixed section `[dbLabCalExt]`. Max. 25 entries are used for the Extra menu.
The section entries are:

```
Program / Document description to be displayed in the Extra menu
 =
full path to program or document with parameter list if applicable for that
particular program/document
```

the parameters will be replaced by dbLabCal with current database values before the called program will be started

```
#databasemodus#
#databasename#

#studyid#
#studycode#
#sponsorcode#
#studycomment#

#peakid#
#peakname#
#matrix#
#analyticalmethod#
#concunit#
#regmodel#
#regweighting#
#regreadings#

#seqid#
#seqnumber#
#sequnit#
#seqcomment#
#seqextracted#
#seqstarted#
#seqended#
#seqcalculated#

#reg_a#
#reg_b#
#reg_c#
#reg_r2#

#selection#

#set_peaknames#
#set_cals#
#set_qcs#
#set_vals#
#set_subjects#
#set_periods#
#set_times#
```

Examples....

```
[dbLabCalExt]
Notepad=c:\windows\notepad.exe

Bug Report (e-mail)=mailto:milan.vagaday@aai.de?Subject=dbLabCal V3 Bug report!
Study:#studycode#
Peak:#peakname#/#matrix#&Body=StudyID=#studyid#PeakID=#peakid#SeqID=#seqid#

New in dbLabCal V3 (PDF-Dokument)=f:\pkg\dblabcal.v3\docs\winidblcV3.pdf
dbLabCal V3 - Manual (PDF-Dokument)=f:\pkg\dblabcal.v3\docs\dblabcalv3de.pdf
Recovery (Excel sheet)=f:\pkg\ExcelSheets\reco.d02.XLT
Recovery with matrix effect for LC/MS (Excel
sheet)=f:\pkg\ExcelSheets\reco_me.d02.xlt
Stability Solutions (Excel sheet)=f:\pkg\ExcelSheets\StabiSol.d03.xlt
Pipettes Calibration (Excel sheet)=f:\pkg\ExcelSheets\PipettenKalib.d01.xlt
Sampler Calibration (Excel sheet)=f:\pkg\ExcelSheets\SamplerKalib.d02.xlt
```

5.6 dblabcal.imp File

dblabcal.imp is a control file for dblabcal.exe. It must be in the same folder as dblabcal.exe
dblabcal.imp is used to describe structure of ASCII file which should be used for data import into the dbLabCal database

In the [Formats] section is a name list of all in the dblabcal.imp defined ASCII formats.
There is no limit for the number of entries in the [Formats] section. The sequence of the entries is arbitrary

The sections must be written exactly as in [Formats] section defined!

e.g.:

```
[Formats]
3=MacQuan(SIEX API300/365)
.
.
[MacQuan(SIEX API300/365)]
column.....=...etc
```

the section entries are:

file_analyte_name=3,1,20	row number, first character, last character (means the analyte name is written in the ASCII file in the 3rd row, between columns 1 – 20 negative row number means row number is counted from the end of the ASCII file
file_analyte_name=-1,1,20	means last row (or first row from the end...)
file_analyte_name=0,...	means, there is no information on the analyte name in the ASCII file
data_after_line_starting_with=#	(data of each chromatogram starts after row #,the first position of chromatogram data is row #+1)
data_before_line_starting_with=#	(data of each chromatogram ends before row # the last position of chromatogram data is row #-1)
data_after_line_starting_with=0	means, the first position of chromatogram data is the first row of ASCII file
data_before_line_starting_with=0	means, the last position of chromatogram data is the last row of ASCII file
column_separator=ASCII code	ASCII code of the column separator character (ASCII code can be a number, e.g. column_separator=9, for TAB or a character , e.g. column_separator=| or column_separator=, etc)
column_filename=	column number, of column containing the chromatogram file name/chromatogram id
column_samplename=	column number, of column containing the sample name
column_rt=	column number, of column containing the retention time of the analyte
column_area=	column number, of column containing the peak area of the analyte
column_ht=	column number, of column containing the peak height of the analyte
column_rtIS=	column number, of column containing the retention time of the internal standard
column_areaIS=	column number, of column containing the peak area of the internal standard
column_htIS=	column number, of column containing the peak height of the internal standard
column_df=	column number, of column containing the sample dilution factor
column_date=	column number, of column containing the date/time of the chromatogram analysis
column_analyte_name=	column number, of column containing the analyte name (with the above measured values) (either file_analyte_name= or column_analyte_name= is possible if file_analyte_name<>0 then column_analyte_name is ignored file_analyte_name<>0 means: 1 file = 1 analyte column_analyte_name<>0 means: 1 file = all analytes of one chrm.run
…	

Example….

```
;dblabcal.imp is a control file for dblabcal.exe
;it must be in the same folder as dblabcal.exe
;it is used to describe structure of ASCII file
;which should be used for data import into dbLabCal database
;-----------------------------------------------------------------
;dblabcal.imp can be used for any (defined) ASCII file format
;-----------------------------------------------------------------
;
;
;in the [Formats] section is a name list of all in the dblabcal.imp
;defined ASCII formats
;there is no limit for the number of entries in the [Formats] section
;
;the following section must be written exactly as in [Formats] section defined!
;
;
;the entries are:
;
;-------------------------------------------------------------------------------------------------------------------
;;data_FirstLine=   OR data_after_line_starting_with= is used
;;special case: data are already in the 1st line, then there were no entry for data_after_line_starting_with possible
;data_FirstLine=
;data_after_line_starting_with=text   (data of each chromatogram starts after row x)
;                                         (the first position of chromatogram data is row x+1)
;data_before_line_starting_with=text  (data of each chromatogram ends before row x)
;                                         (the last position of chromatogram data is row x-1)
;data_after_line_starting_with=0 means, the first position of chromatogram data is the first row of ASCII file
;data_before_line_starting_with=0 means, the last position of chromatogram data is the last row of ASCII file
;
;data_ignore_if_name=text means don't import this line if sample name column content is "text", used for Magellan
;
;
;data_project=row, col
;data_unit_name=row, col
;data_batch_number=row, col
;data_batch_comment=row, col          (used for FACS)
;data_batch_user=row, col             (used for FACS)
;data_extraction_date=row, col
;data_start_date=row, col             (used for FACS)
;data_end_date=row, col
;
;
;column_separator=ASCII code of the column separator character (for example column_separator=9, for TAB)
;                 or the character (for example column_separator=|, column_separator=, column_separator=;)
```

```
;-------------------------------------------------------------------------------------------------------------------------------
;
;
;1file_1peak=                    1 if 1file = 1peak, 0 if 1file=all peaks from a chromatogram
;-------------------------------------------------------------------------------------------------------------------------------
;if 1file_1peak=1
;file_analyte_name=     row number, first character, last character
;file_analyte_name=3,1,20 means the analyte name is written in the ASCII file in the 3rd row, between the columns 1 and 20)
;
;negative row number means row number counted from the end of the ASCII file
;file_analyte_name=-1,1,20 means last row (or first row from the end...)
;file_analyte_name=0,...   means, there is no information on the analyte name in the ASCII file
;
;
;column_filename=       column number, of column containing the chromatogram file name/chromatogram id
;column_samplename=     column number, of column containing the sample name
;column_rt=             column number, of column containing the retention time of the analyte
;column_area=           column number, of column containing the peak area of the analyte
;column_ht=             column number, of column containing the peak height of the analyte
;column_rtIS=           column number, of column containing the retention time of the internal standard
;column_areaIS=         column number, of column containing the peak area of the internal standard
;column_htIS=           column number, of column containing the peak height of the internal standard
;column_df=             column number, of column containing the sample dilution factor
;column_date=           column number, of column containing the date/time of the chromatogram analysis
;column_analyte_name=   column number, of column containing the analyte name (with the above measured values)


;column_samplename_starts_after= last! character(s) after which the sample name starts (within the column "column_samplename")
                                                    if empty, sample name starts at position 1 of the column
"column_samplename"
;column_samplename_ends_before=  first! character(s) before which the sample name ends (within the column "column_samplename")
                                                    if empty, sample name ends with the end of the whole column
"column_samplename" content


;column_sampletype=     column number, of column containing CAL, QCS, VAL, SUB, DIV, KON
;column_sampleinfo=     column number, of column containing DIVtext, SUB##, , SUB#######
;column_sampleperiod=   column number, of column containing period for SUB ##
;column_sampletime=     column number, of column containing time for SUB VAL
;column_samplematrix=   column number, of column containing for VAL
;column_sampletemp=     column number, of column containing for VAL
;column_nomconc=        column number, of column containing CAL, QCS, VAL
;column_samplecomment=  column number, of column containing comment
;-------------------------------------------------------------------------------------------------------------------------------
;
;columns for Magellan (double assays)
;*.asc
```

```
;column_samplename2=
;column_readings=
;column_values=
;column_calcconcMEAN=
;column_calcconcCV=
;column_calcconcDEV=
;MEAN, DEV, SD, CD are imported from Magellan
;
;columns for Access2 (double assays)
;*.csv
;column_samplename is Patienten-ID
;column_filename is   Proben-ID
;column_calcconc is   Ergebnis
;column_values is     RLU
;column_calcconc
;column_date
;MEAN, DEV, CV are calculated in dbLabCal
;-------------------------------------------------------------------------------------------------------------------------
;
;if 1file_1peak=1       peaks in own ASCII file
;AND column_analyte_name=x,y(,z)peak name position (McQuan)
;
;
;if 1file_1peak=0       all peaks from a chromatogram in ONE ASCII file
;AND column_analyte_name=0            in different columns (FACS)
;
;or
;if 1file_1peak=0       all peaks from a chromatogram in ONE ASCII file
;AND column_analyte_name=x            in one column (Analyst, Millennium)
;
;-------------------------------------------------------------------------------------------------------------------------
;-------------------------------------------------------------------------------------------------------------------------
;;analyte name is in row as defined in "data_after_line_starting_with="
;-------------------------------------------------------------------------------------------------------------------------
;column_analyte_name01= column number, of column containing the name of peak 1
;column_analyte_name02= column number, of column containing the name of peak 2
;column_analyte_name03= column number, of column containing the name of peak 3
;etc...
;column_analyte_name10= column number, of column containing the name of peak 10
;-------------------------------------------------------------------------------------------------------------------------
; OR
;-------------------------------------------------------------------------------------------------------------------------
;;analyte name is in specific row, col
;-------------------------------------------------------------------------------------------------------------------------
;column_analyte_name01= row, column number, containing the name of peak 1
;column_analyte_name02= row, column number, containing the name of peak 2
;column_analyte_name03= row, column number, containing the name of peak 3
```

```
;etc...
;column_analyte_name10= row, column number, containing the name of peak 10
;-------------------------------------------------------------------------------------------------------------------------
;-------------------------------------------------------------------------------------------------------------------------
;
;
;column_rt01=           column number, of column containing the retention time of peak 1
;column_area01=         column number, of column containing the peak area of peak 1
;column_ht01=           column number, of column containing the peak height of peak 1
;column_rtIS01=         column number, of column containing the retention time of the internal standard for 1
;column_areaIS01=       column number, of column containing the peak area of the internal standard for 1
;column_htIS01=         column number, of column containing the peak height of the internal standard for 1
;column_nomconc01=      column number, of nomical conc. for Peak01
;
;column_rt02=           column number, of column containing the retention time of peak 2
;column_area02=         column number, of column containing the peak area of peak 2
;column_ht02=           column number, of column containing the peak height of peak 2
;column_rtIS02=         column number, of column containing the retention time of the internal standard 2
;column_areaIS02=       column number, of column containing the peak area of the internal standard 2
;column_htIS02=         column number, of column containing the peak height of the internal standard 2
;column_nomconc02=      column number, of nomical conc. for Peak02
;
;etc..
;
;column_rt10=           column number, of column containing the retention time of peak 10
;column_area10=         column number, of column containing the peak area of peak 10
;column_ht10=           column number, of column containing the peak height of peak 10
;column_rtIS10=         column number, of column containing the retention time of the internal standard 10
;column_areaIS10=       column number, of column containing the peak area of the internal standard 10
;column_htIS10=         column number, of column containing the peak height of the internal standard 10
;column_nomconc10=      column number, of nomical conc. for Peak10
;
;
;-------------------------------------------------------------------------------------------------------------------------
;
;dblabcal.imp-Format-Description-END
;-----------------------------------------------
```

```
[Formats]
1=*.csv (FACS) nocalc

[*.csv (FACS) nocalc]
column_separator=,

1file_1peak=0
file_analyte_name=0

data_project=
data_unit_name=
data_batch_number=
data_batch_comment=
data_batch_user=
data_extraction_date=
data_start_date=
data_end_date=

data_analyte_name01=1,3
data_analyte_name02=1,5
data_analyte_name03=1,7
data_analyte_name04=1,9
data_analyte_name05=1,11
data_analyte_name06=1,13
data_analyte_name07=1,15
data_analyte_name08=1,17
data_analyte_name09=1,19
;data_analyte_name10=1,21

data_after_line_starting_with=_TAB_Sample ID
;data_before_line_starting_with=

column_analyte_name01=1,3
column_analyte_name02=1,5
column_analyte_name03=1,7
column_analyte_name04=1,9
column_analyte_name05=1,11
column_analyte_name06=1,13
column_analyte_name07=1,15
column_analyte_name08=1,17
column_analyte_name09=1,19
column_analyte_name10=1,21
;if column NN doesn't exist the PeakCount is automatically corrected...
```

```
column_filename=0
column_samplename=2
column_samplename_starts_after=
column_samplename_ends_before=

column_df=0

column_area01=4
column_ht01=

column_area02=6
column_ht02=

column_area03=8
column_ht03=


column_area04=10
column_ht04=


column_area05=12
column_ht05=

column_area06=14
column_ht06=

column_area07=16
column_ht07=

column_area08=18
column_ht08=


column_area09=20
column_ht09=

column_area10=22
column_ht10=
```